



Users Guide for the Program TAMDYN. A Modelling Tool for Use on Personal Computers to Simulate Environmental Transport of Contaminants

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Users Guide for the Program TAMDYN

A modelling tool for use on personal computers to simulate environmental transport of contaminants

Béla Kanyár and Sven P. Nielsen

RISØ-M-2741

USER'S GUIDE FOR THE PROGRAM TAMDYN

A modelling tool for use on personal computers to
simulate environmental transport of contaminants

Béla Kanyár* and Sven P. Nielsen

Abstract. Recent developments in radioecology have stressed the need for providing uncertainties associated with model predictions. Our aim was to get a flexible computer program to estimate these uncertainties even for dynamic processes, and mainly for time-dependent solutions of compartmental systems. Therefore, we have combined the uncertainty analysis code TAM3 (written by R. H. Gardener, Oak Ridge National Laboratory, USA) and the code of RKF45 for integration of ordinary differential equations by the Runge-Kutta-Fehlberg method. The source program of TAM3 is written in Turbo Pascal for PC-computers and so is the present extension for dynamic systems.

The structure of the compartmental system (number of compartments, non-zero transfer coefficients etc.) can be defined from the input data. The extension to dynamic systems includes an option to modify the values of the state variables and non-transfer parameters during the solution of the differential equations. The modifications are given in the input data and are useful for the simulation of contaminations, harvesting etc.

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1. INTRODUCTION

In validation studies of models used to simulate transport of radionuclides in the environment it is essential to estimate the variations of the model predictions associated with the uncertainties of the parameters and modelling processes. To provide uncertainties, one of the most common methods is the Monte Carlo simulation (IAEA, 1988). This method is implemented in the computer code TAM3 for models of steady-state compartmental systems, written by R. H. Gardner (Gardener, 1988). The advantages of the code which runs on personal computers under DOS are the following:

- the user-friendly menus, from where it is easy to specify and modify the parameters, provide deterministic solutions, sensitivity and uncertainty analyses,
- possibility to specify correlations among the parameters.

In the present form of program TAM3, the model specifications (number of compartments, non-zero matrix elements etc.) are given in a subroutine. But to change the program from one problem to the other involves re-programming, even though in Turbo Pascal it is easy to change the program and compile it again. Therefore, our first modification was to write a procedure for constructing the system-matrix and the output functions from an input data file. This way it is easy to change the model and the problem.

To extend the program for dynamic compartmental systems (time dependent solutions) we have added the procedure of the Runge-Kutta-Fehlberg method (Fehlberg, 1977) to integrate the differential equations. The user defines the initial values of the state variables and the timepoints at which outputs are wanted either for deterministic solutions or uncertainty analyses.

The extension to dynamic systems contains a possibility to modify the values of the state variables and non-transfer parameters during the solution of the differential equations. The modifications are given by the input data and are called as discrete events. These are useful for the simulation of prolonged con-

taminations, harvesting etc.

A more general and flexible program for an uncertainty analysis and the fitting of even dynamic models associated with radio-nuclide transfer has been developed by T. B. Kirchner (Kirchner, 1987). Kirchner has used the fourth-order Runge-Kutta method to solve the differential equations. In the case of a stiff problem, the Fehlberg modification implemented by us might be more efficient. The comparison of the two procedures is planned in the future.

In the case of nonlinear compartmental systems, a general formulation is usually impossible and/or less effective, and for this case the user has to modify the source program and add the written procedure to the program.

2. USERS GUIDE

The program TAMDYN (an extension of the TAM3 uncertainty analysis program to dynamic systems) is written in Turbo Pascal and the executable code is TAMDYN.COM. The source codes are given in the files of

- TAMD.PAS (main program)
- MENUUD.INC (operates the program menu)
- MATRIXD.INC (solves the steady-state system by matrix inversion)
- INITD.INC (reads and initializes the parameters)
- DYN SOL.INC (solves the dynamic system)
- STATSD.INC (statistical analysis)
- MVRNGD.INC (random number generator).

2.1. Input Parameters

Table 1 shows an example of the ASCII file for input data. This file can be made with a suitable editor. The first line contains the title of the problem (maximum 40 characters). The second depends on the program branching. If the model is a linear compartmental system with constant coefficients (either a steady-state or dynamic one) the data are the following:

- ndim : number of the compartments (dimension of the system)
- ntr : number of the non-zero transfer coefficients
- npar : number of the parameters used in the uncertainty analysis
- ncons : number of the constants used (for the case of a user written procedure)
- nstates: number of states (outputs) defined by use of the state variables and non-transfer (secondary) parameters.

For non-compartmental models (e.g. an algebraic function in explicit form) only the last three parameters are to be written into the data file (see Table 2).

Table 1. Input data file for a compartmental system.

testdata-tam-riso DYNAM	
3 7 12 0 4	{ndim, ntr, npar, ncon, nstates}
watr sedi fish	{names of compartments}
envi>watr n 2.592e+8 2.58e7 0. 1.0e30	{transf.coeffs: defin.
watr>sedi n 1.288e-3 1.29e-4 0. 1.0e30	{distr.
sedi>watr n 8.83e-7 8.8e-8 0. 1.0e30	{mean
sedi>envi n 5.48e-4 5.5e-5 0. 1.0e30	{st. dev.
watr>fish n 4.06e-11 4.1e-12 0. 1.0e30	{minimum
fish>watr n 3.40e-4 3.4e-5 0. 1.0e30	{maximum}
watr>envi n 2.742e-3 2.7e-4 0. 1.0e30	
sdil n .5 .05 0. 1.0e30	{secondary
crcf n .01 .001 0. 1.0e30	{parameters}
wama n 1.36e11 1.36e10 0. 1.0e30	
sema n 3.57e7 3.57e6 0. 1.0e30	
fima n 1.64e3 1.64e2 0. 1.0e30	
waterconc :=watr/wama.	{output
sedimconc :=sedi/sema.	
fishconc :=fish/fima.	{functions
crops :=sedi*sdil/sema*crcf.	
0.0 1.0 0.0 0.0	{init. values for dynam. system: t and y[i]}
watr 1000. 0.3	{ event: code, time, factor}
EEEE	{ end of events}

Table 2. Input data file showing a user-written model and the use of constants.

Test-data for user-written model	{ title of problem
4 3 2	{ npar, ncon, nstates
	{ parameters
alco 1 80. 30. 20 120	
a2co 1 20. 10. 1.0 50.	
lam1 n -0.20 0.1 -1.0 -0.05	
lam2 n -0.03 0.03 -0.2 -0.001	
10.2 1.0 3	{ constants
activity1	{ names of output
activity2	{ functions

The third line contains the names of the compartments (state variables) if `ndim > 0`. The length of the names are fixed to four characters separated by a single space.

The parameters are defined - in our first example - from the beginning of the 4th line. If `ntr > 0` the non-zero transport coefficients are defined by the names of the two connected compartments. Between the names is placed the character of `>` (greater than) and the environment is named as "envi".

After the definition of the transport coefficients the 11. column specifies the type of distribution of the parameter (`n:normal`, `l:lognormal`, `u:uniform`, `g:loguniform`, `t:triangular`, `r:logtriangular` and `c:constant`). The mean value, the standard deviation, the lower and upper limits are given on the same line as the distribution specification. (For a constant only the "mean" value is read in.)

The name of secondary parameters (if `npar > ntr`) are defined in the same form as the transfer coefficients. These names may contain up to 9 characters, but only the first 4 are used for identification. Be careful!

For `ncons > 0` (only for a model procedure written by the user) the values of the constants are given after the parameter definitions in free format with at least one space as delimiter, and without any names.

The output functions (states, responses etc.) are given following the parameters or constants if $ncons > 0$. The length of the names may contain up to 9 characters and all 9 are used for identification. In the definition (after the assignment operator $:=$), the names of compartments and non-transfer parameters can be used in combination with the four basic arithmetic operators $+$, $-$, $*$ and $/$. The maximum number of names in one definition is 9. The output functions are always terminated at the end of the line with a period, and they have to be started from the beginning of a new line.

For a user-written function, the output definitions must be placed inside the user procedure, and only the names of the functions are written into the input data file (see Table 2).

The next input data are only for dynamic systems. First, the starting value of the time (t) and then the initial values of the state variables (the amount of radioactivity or other quantities in the compartments) in free format.

The definitions of the discrete events are to be written line-by-line in the following form:

- name of quantity (state variable or secondary parameter) to be modified (four character length),
- date of modification (units the same as the running time),
- modifying factor (the quantity is multiplied by this factor).

The new value is valid until there is any new modification. In case where simulations are repeated (uncertainty analysis) the initial values of the state variables and the parameters are stored for a new run and the effects of the events are repeated.

2.2. The Menu and Executing the Program

The first menu displayed after starting is given in Figure 1. The choices are the same as in the code TAM3, except for the first three.

Program Control:

- <W> Model given by a Written proc.
- <X> Steady-State compartment
- <Y> Dynamic compartment
- <C> Read, change and save variables

Program Execution:

- <D> Deterministic Solution
- <S> Sensitivities
- <M> Monte Carlo Analysis

Display Results:

- <V> Untransformed Statistics
- <L> Log-transformed Statistics
- <P> Print
- <Z> Set Statistics to Zero

Exit Program:

- <Q> Quit

Figure 1. Screen of the Initial Menu

2.2.1. Keys of Program Control

W : You wish to use a previously written, compiled and linked model-procedure (from the next display you have to chose the proper model A, B or C etc. The choices of X, Y and W must

not be used there).

X : The model is defined as a steady-state compartmental system.

Y : The model is defined by a set of differential equations (dynamic model) and the time-dependent solutions are used. Even for a user-written dynamic model the choice of Y is to be used (and not W). But in this case the number of the transfer coefficients must be zero ($ntr = 0$) and the execution turns to the user procedure named "DynamUser".

C : To modify the parameters of the model or/and program the menus shown in Figures 3-7 can be used.

<L> Load Model and/or Parameters from Disk File

<E> Edit Parameter Values and Statistics

<C> Correlate Parameters

<S> Save Parameters to Disk File

<P> Print Parameters

<V> Change Program Variables

<T> For dynamic system give or change the times

<R> Return

Figure 2. Screen of the Menu of the Modifications

2.2.2. Keys of Program Execution

Following the editing of the model parameters and/or the time data (for dynamic cases) the user has to choose between the deterministic (D), sensitivity (S) and uncertainty (M) analysis.

In the dynamic case the user has to give the step size and (increasing) time points to the questions on the screen. These data are not stored in the data file and cannot be written onto it. For deterministic solutions the outputs are stored stepwise according to the fixed step size entered formerly. The integration is performed until the last time point. The S and M analyses are made at the dates (time points) entered formerly.

In all the three cases (D,S,M) the user is asked whether the results are to be stored on disk, printed or displayed. In case of disk storage the output file names must be given. The results of simulations (time, predicted state variables and defined output functions) are stored on the disk file together with the sensitivity and uncertainty analysis reports, but not the correlation coefficients. Therefore, if the correlations among all the possible random variables are important, they have to be printed after each date. It means that in this case only one date is to be given for sensitivity and uncertainty calculations. After printout of the correlations the calculations can start with the next date.

testdata-tam-riso DYNAM

The t-values to modify them

step : 100.000

1: 500.000

2: 2000.000

3: 10000.000

Figure 3. Modification of the time points (only for dynamic systems)

Number	Name	Mean	Dist	St.Dev	Minimum	Maximum
1	envi>watr	2.59E+08	N	2.58E+07	0.00E+00	1.00E+30
2	watr>sedi	1.29E-03	N	1.29E-04	0.00E+00	1.00E+30
3	sedi>watr	8.83E-07	N	8.80E-08	0.00E+00	1.00E+30
4	sedi>envi	5.48E-04	N	5.50E-05	0.00E+00	1.00E+30
5	watr>fish	4.06E-11	N	4.10E-12	0.00E+00	1.00E+30
6	fish>watr	3.40E-04	N	3.40E-05	0.00E+00	1.00E+30
7	watr>envi	2.74E-03	N	2.70E-04	0.00E+00	1.00E+30
8	sdil	5.00E-01	N	5.00E-02	0.00E+00	1.00E+30
9	crcf	1.00E-02	N	1.00E-03	0.00E+00	1.00E+30
10	wama	1.36E+11	N	1.36E+10	0.00E+00	1.00E+30
11	sema	3.57E+07	N	3.57E+06	0.00E+00	1.00E+30
12	fima	1.64E+03	N	1.64E+02	0.00E+00	1.00E+30

Distributions: <N>ormal <L>ogNorm <U>niform <C>onstant
 <T>riangular lo<G>uniform logt<R>iangular

Type number of parameter to edit - or 0 to return

Figure 4. Screen for modifying the model parameters.

Correlations Between Model Parameters					
Index	Parameter	with	Index	Parameter	Correlation
1	envi>watr				
2	watr>sedi				
3	sedi>watr		2	watr>sedi	0.9500
4	sedi>envi				
5	watr>fish				
6	fish>watr				
7	watr>envi				
8	sdil				
9	crcf				
10	wama				
11	sema				
12	fima				

Figure 5. Screen for setting the correlation coefficients

The modification procedure of the model parameters, correlation coefficients etc. is the same as in the TAM3 (Figures 4-6) and in the same way we have added the input procedure of the time points (Figure 3).

2.2.3. Keys of display of the results.

The output of the statistical calculations (mean values, standard deviations, correlations etc.) achievable by the key V are the same as in TAM3. Modifications are made only in the output formats.

Program Control Variables

1 **Printer OFF**

2 **Untransformed statistics only**

3 **Time: 11:24 am**

4 **Date: 05/19/1988**

5 **Title: testdata-tam-riso DYNAM**

6 **Iterations: 100**

Type number of variable to change - or 0 to return

Figure 6. Screen for setting the program control parameters.

2.3. Output Results

The Figures 7-10 show results of the steady-state solution from the model defined by the input data given as an example.

The results of the deterministic solution for the dynamic case of the model defined by the data of the example are given in Figure 11.

Steady-State Solution of testdata-tam-riso DYNAM

waterconc	sedimconc	fishconc	crops	water	sed	fish
4.732E-01	4.230E+03	4.686E+00	2.115E+01	6.435E+10	1.510E+11	7.684E+03

Figure 7. Deterministic solution of the steady-state case. In addition to the output functions (the concentrations) for the deterministic case the amounts of the compartments are printed, too.

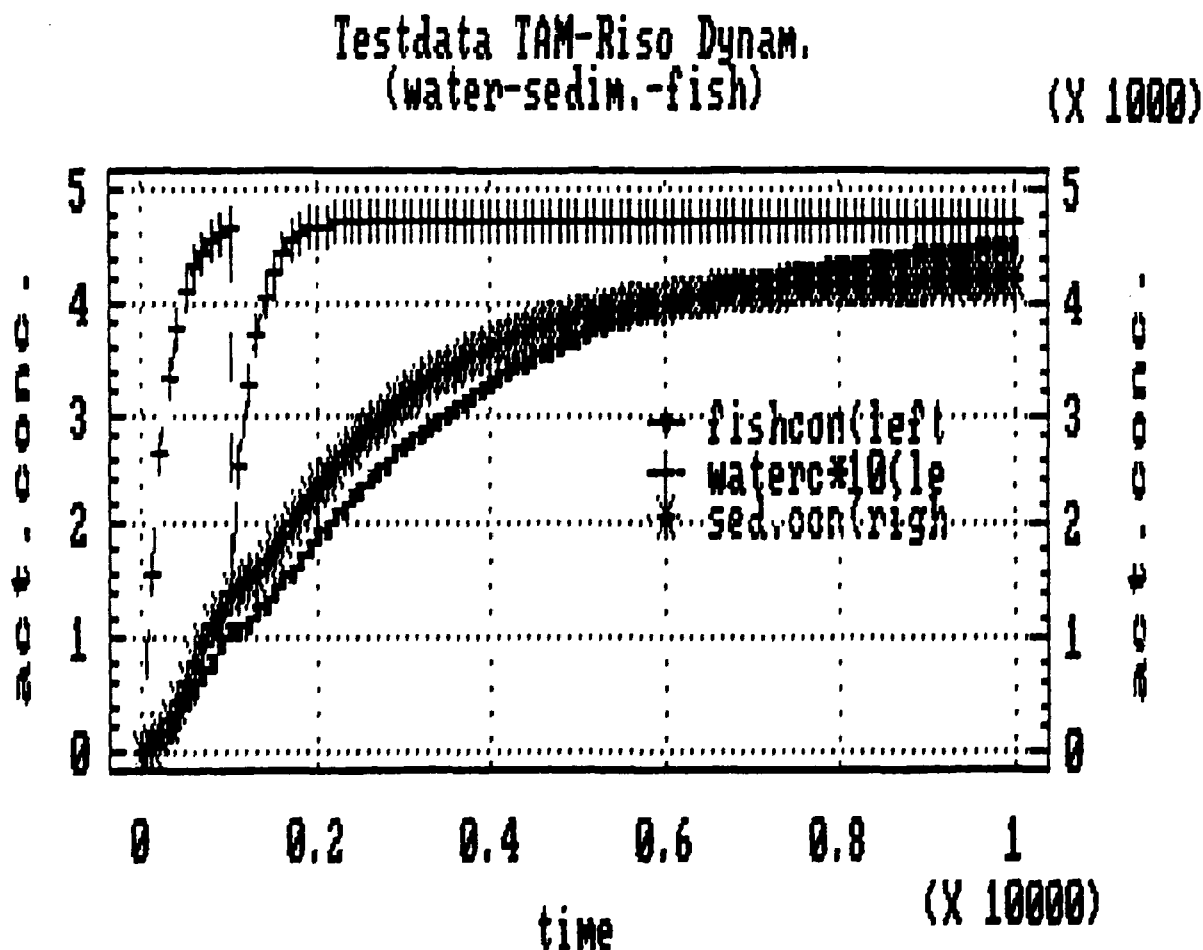


Figure 8. Deterministic solution of the dynamic (time-dependent) case. The output of the TAMDYN is written to a diskfile (type .dat). One variable needs 10 characters (width), the first column is the time and the first row contains the names of the variables. (The plot is made with STATGRAPHICS.)

Monte Carlo Analysis of testdata-tam-riso DYNAM

ncnt= 20

variables have not been log-tranformed

	waterconc	sedinconc	fishconc	crops
envi>watr	41.47	7.37	5.32	13.23
watr>sedi	7.16	2.11	0.55	0.45
sedi>watr	0.97	4.38	1.84	3.49
sedi>envi	6.73	41.82	0.44	26.77
watr>fish	0.05	4.01	40.05	6.00
fish>watr	0.36	20.15	16.90	29.46
watr>envi	1.52	7.78	3.84	0.83
sdil	5.68	5.43	2.80	33.46
crcf	6.07	0.51	13.37	32.27
wama	72.96	3.25	3.00	0.08
sema	8.19	2.26	7.65	0.11
fima	17.58	7.74	21.70	7.85
totals=	168.7	106.8	117.5	154.0

Hit any key to continue

Figure 9. Results of the uncertainty analysis for the steady-state solution. (ncnt: number of sampling or iterations; for most of the real situations ncnt > 100 gives reasonable statistical results.)

Percent Sensitivity Analysis of testdata-tam-riso DYNAM

ncnt=	20			
	waterconc	sedimconc	fishconc	crops
envi>watr	54.36	17.56	27.71	5.58
watr>sedl	24.98	5.51	0.10	3.42
sedl>watr	3.63	25.52	9.25	9.49
sedl>envi	0.49	15.74	1.98	0.13
watr>fish	4.26	31.08	33.89	10.42
fish>watr	2.36	29.58	0.98	1.10
watr>envl	1.62	23.91	13.03	29.36
sdil	1.78	4.27	0.03	9.85
crcf	2.38	1.89	0.55	20.39
wama	43.38	0.16	8.63	3.76
sewa	3.65	12.84	0.25	13.03
fima	0.09	14.55	27.52	11.53
totals=	143.0	182.6	123.9	118.1

Hit any key to continue

Figure 10. Results of sensitivity analysis for the steady-state solution.

Monte Carlo Analysis of testdata-tam-riso DYNAM

ncnt= 20 t= 3.0000E+02

correlations specified and variables have not been log-transformed

	waterconc	sedimconc	fishconc	crops
envi>watr	56.37	49.86	30.74	14.80
watr>sedi	1.28	17.80	0.85	46.76
sedi>watr	0.88	17.84	1.18	34.96
sedi>envi	11.12	0.07	30.33	0.14
watr>fish	0.02	0.02	22.64	7.54
fish>watr	8.04	8.84	1.22	0.97
watr>envi	4.38	1.09	1.18	2.62
sdil	1.05	1.50	1.54	20.55
crcf	2.81	23.30	19.31	0.49
wama	65.38	0.01	0.00	1.57
sema	1.77	38.50	0.26	3.07
fima	5.73	0.03	42.17	3.76
totals=	158.8	158.9	151.4	137.2

Hit any key to continue

Figure 11. Results of the uncertainty analysis for the dynamic solution at t=300.

Monte Carlo Analysis of testdata-tam-riso DYNAM

ncnt= 20 t= 1.0000E+04

correlations specified and variables have not been log-tranformed

	waterconc	sedimconc	fishconc	crops
envi>watr	47.43	27.67	23.40	18.97
watr>sedi	0.47	8.07	3.06	2.77
sedi>watr	2.19	4.83	0.75	4.03
sedi>envi	0.53	46.89	0.36	27.29
watr>fish	0.24	1.12	0.13	9.28
fish>watr	2.43	0.95	28.42	6.00
watr>envi	5.25	2.05	6.86	0.11
sdil	4.73	2.07	7.59	26.09
crcf	22.87	20.78	0.45	0.69
wama	26.03	1.03	21.30	5.67
sema	1.60	22.14	0.23	20.06
fima	0.78	6.57	57.22	9.93
 totals=	 114.6	 144.2	 149.8	 130.9

Hit any key to continue

Figure 12. Results of uncertainty analysis for the dynamic solution at t=10000 (near steady-state).

Frequency Histogram of the sedim. conc. in steady-state

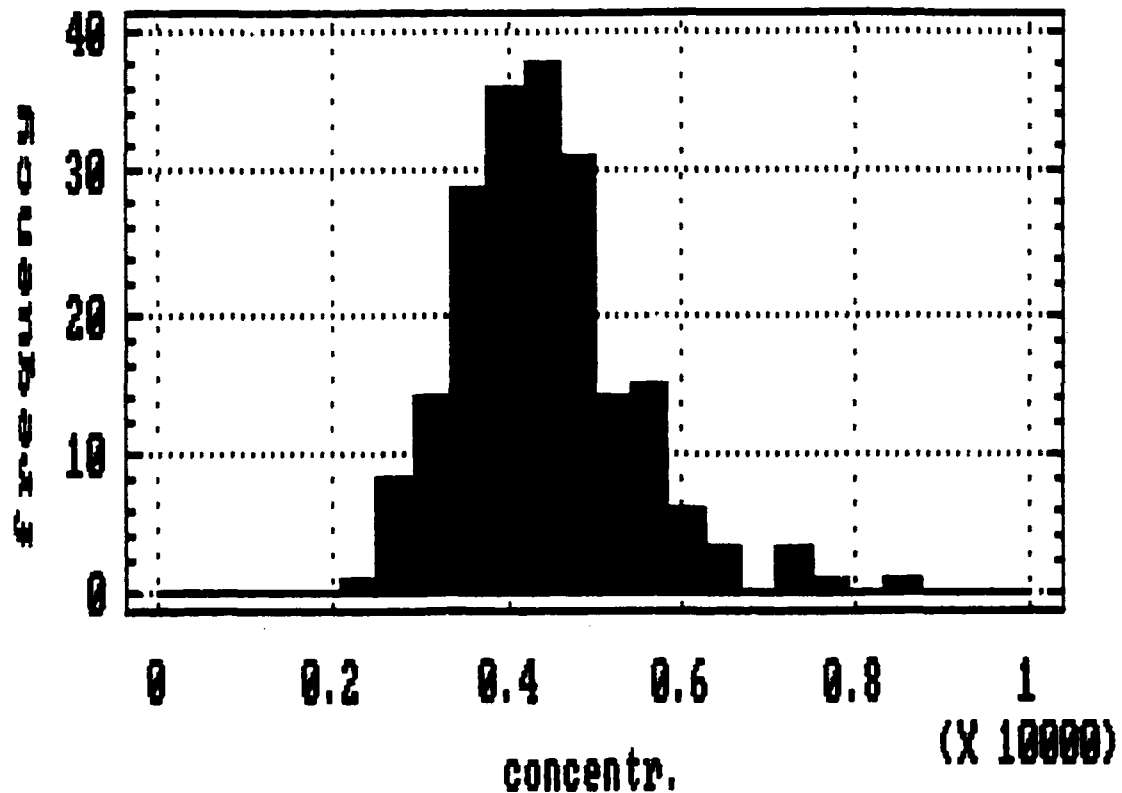


Figure 13. Frequency distribution of the results for the steady-state solution of the data example (ncnt=100); plot made with STATGRAPHICS.

From the analysis reports of the same run but at different time points the results can be rearranged and plotted for separate parameters with respect to time. Such a plot is shown in Figure 15.

2.4. Structure of the program

The whole program comprises about 2200 lines and contains more than 30 procedures. The procedures for statistical analysis and steady-state solution of the compartmental systems are used from the code TAM3. The main procedures and the branchings of the execution are shown in the figures 16 and 17.

ARITHMETIC MEANS AND STANDARD DEVIATIONS

Sample size = 200

Variable	Mean	Std Dev	Minimum	Maximum	C.V.
envi>watr	2.58E+08	2.48E+07	1.88E+08	3.23E+08	9.60 %
watr>sedi	1.29E-03	1.23E-04	9.99E-04	1.66E-03	9.52 %
sedi>watr	8.77E-07	8.84E-08	6.56E-07	1.11E-06	10.07 %
sedi>envi	5.41E-04	5.36E-05	3.88E-04	7.03E-04	9.91 %
watr>fish	4.10E-11	3.95E-12	3.11E-11	5.10E-11	9.63 %
fish>watr	3.41E-04	3.72E-05	2.50E-04	4.37E-04	10.92 %
watr>envi	2.70E-03	2.93E-04	1.99E-03	3.45E-03	10.49 %
sdil	4.99E-01	5.11E-02	3.74E-01	6.29E-01	10.23 %
crcf	1.01E-02	1.07E-03	6.47E-03	1.27E-02	10.56 %
wama	1.37E+11	1.41E+10	1.01E+11	1.73E+11	10.33 %
sema	3.60E+07	3.54E+06	2.73E+07	4.42E+07	9.81 %
fima	1.65E+03	1.70E+02	1.17E+03	2.09E+03	10.31 %
waterconc	4.82E-01	8.59E-02	2.90E-01	7.57E-01	17.82 %
sedimconc	4.39E+03	9.02E+02	2.29E+03	6.95E+03	20.54 %
fishconc	4.88E+00	1.19E+00	2.78E+00	8.78E+00	24.47 %
crops	2.22E+01	5.80E+00	9.16E+00	4.85E+01	26.15 %

Show/write correlations <Y,N>

Show/write correlations <Y,N>

Correlation Matrix

	envi>watr	watr>sedi	sedi>watr	sedi>envi	watr>fish
envi>watr	1.0	0.069	-0.009	-0.019	0.082
watr>sedi	0.069	1.0	0.005	-0.020	-0.058
sedi>watr	-0.009	0.005	1.0	-0.015	-0.084
sedi>envi	-0.019	-0.020	-0.015	1.0	-0.073

Figure 14. Statistical results of the uncertainty analysis (mean values etc., and correlations from part of the output) for the steady-state case.

Testdata TAM-Riso Dynam.
(param.uncert.in time duration)

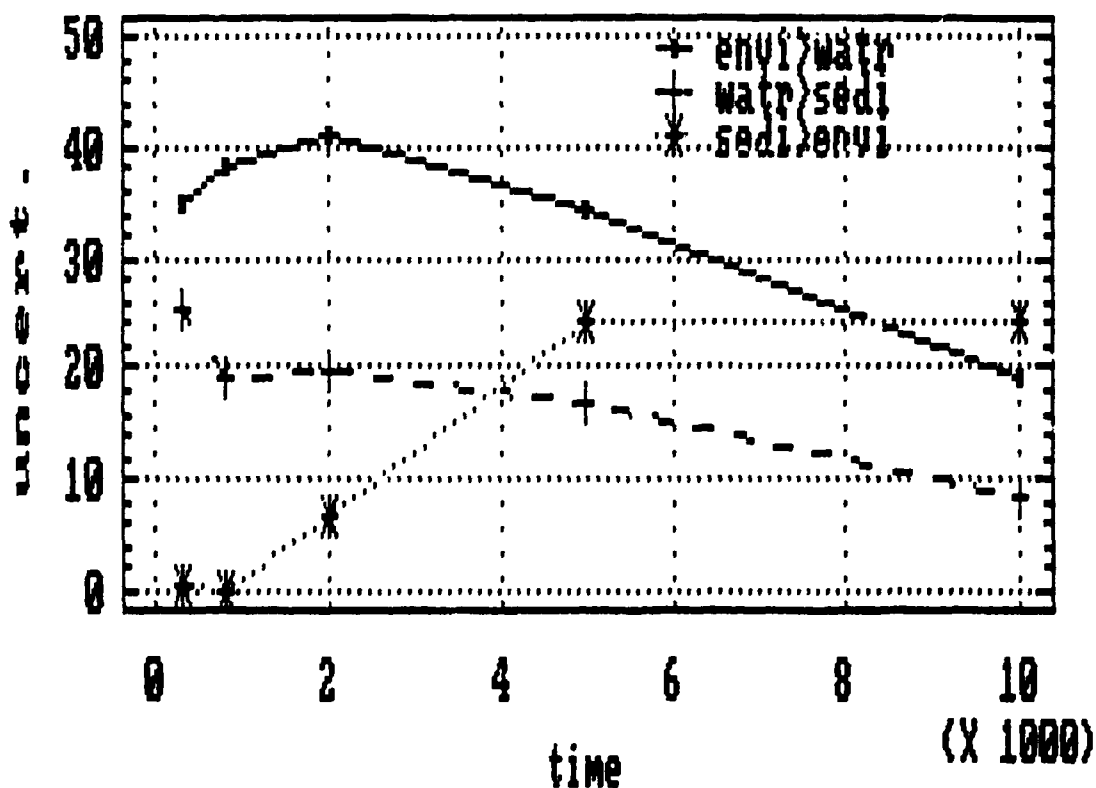


Figure 15. Changes of the relative contributions of dominant parameter uncertainties to the uncertainty of the output function with respect to time. The output function is the sediment concentration and the sampling size, ncnt = 100.

Mc: modelcode

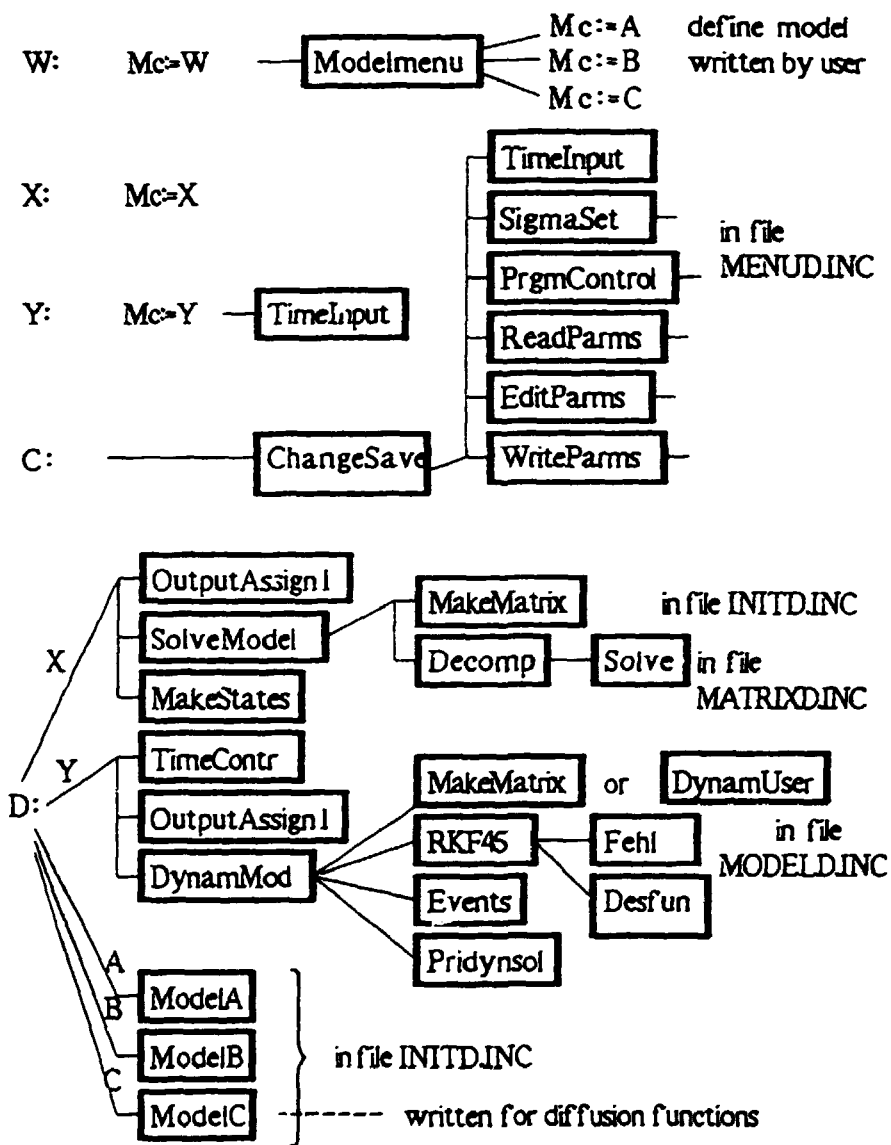


Figure 16. The main procedures and a schematic flowchart for the cases of

- W : user-written procedure
- X : steady-state compartments
- Y : dynamic system
- D : deterministic solution

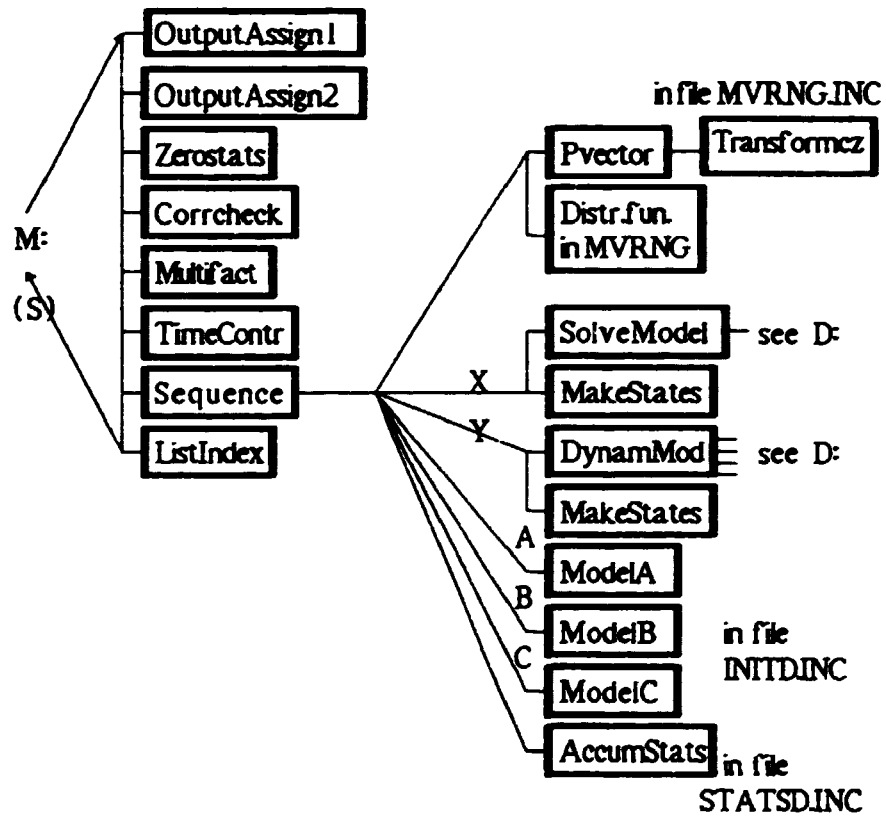


Figure 17. The main procedures used for the uncertainty (M) and sensitivity (S) analyses.

3. PROGRAM PARAMETERS

The present version of the code is developed for the PC computers. The text of the source program in Turbo Pascal needs 45 kbytes and the data 55 kbytes. By these memory sizes the limitations are the following:

- dimension of the differential equation system: 17
- number of model parameters : 35
- number of the output functions (states) : 10
- number of the constants : 50
- number of the events : 50 .

The largest part of the computer memory is used for the statistical matrix (correlation coefficients) by a two-dimensional array of $(npar+nstate)*(npar+nstate)$.

The running time of our example water-sediment-fish problem is nearly 1 sec in case of the deterministic solution of the steady-state system (three compartments) on an Olivetti-PC, model M-24 with a mathematical co-processor. The dynamic solution for the same problem at time intervals 0-10000, with stepsize 100 needs 50 sec. By variation of the stepsize for the output frequency and the precision of integration (now we have used 0.001 as the absolute and 0.02 as the relative error in the procedure RKF45) the running time may be changed by a factor of 3-5. In general the running time is proportional to the square of the number of compartments and for a model with 12 equations and time-dependent transfer coefficients we have got 10-20 min depending on the time-interval of the dynamic system.

4. REFERENCES

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Title and author(s) USERS GUIDE FOR THE PROGRAM TAMDYN A modelling tool for use on personal computers to simulate environmental transport of contaminants. Béla Kanyár* and Sven P. Nielsen *Present adress: National Institute of Radiobiology and Radiohygiene, Budapest, Hungary	Date March 1988
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Abstract (Max. 2000 char.) Recent developments in radioecology have stressed the need for providing uncertainties associated with model predictions. Our aim was to get a flexible computer program to estimate these uncertainties even for dynamic processes, and mainly for time-dependent solutions of compartmental systems. Therefore, we have combined the uncertainty analysis code TAM3 (written by R.H. Gardener, Oak Ridge National Laboratory, USA) and the code of RKF45 for integration of ordinary differential equations by the Runge-Kutta-Fehlberg method. The source program of TAM3 is written in Turbo Pascal for PC-computers and so is the present extension for dynamic systems. The structure of the compartmental system (number of compartments, non-zero transfer coefficients etc.) can be defined from the input data. The extension to dynamic systems includes an option to modify the values of the state variables and non-transfer parameters during the solution of the differential equations. The modifications are given in the input data and are useful for the simulation of contaminations, harvesting etc.	
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